
Article:
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Erratum: Improved real-space genetic algorithm for crystal structure and polymorph prediction [Phys. Rev. B 77, 134117 (2008)]

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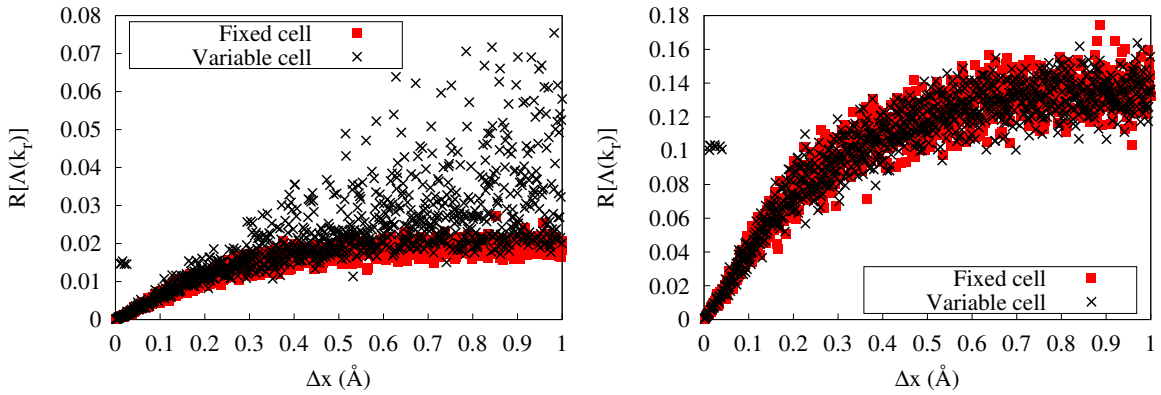
In the original paper, there was an error in the derivation of the spherically averaged scattering intensity, presented in Eq. (5) in the original paper. This equation should have read:

$$\Lambda\left(k_r\right) = \sum_{n=1}^{N} \rho'(n)^2 + 2\sum_{n=1}^{N}\sum_{m>n}^{N} \rho'(n)\rho'(m) j_0\left(k_r\left|\mathbf{r}_n - \mathbf{r}_m\right|\right) \tag{1}$$

where $j_0(r)$ is the spherical Bessel function of the 1st kind.

The consequence of using the incorrect equation is that the R-factor behaved significantly differently for calculations with varying volumes, and also had an imbalance between the two terms which skewed the results.

Figure 1 shows the R-factor when comparing a reference 8-atom silicon unit cell to a perturbed copy of that cell. In the replica, the atomic positions, and optionally cell vectors, have been randomly perturbed up to some amount Δx. The original equation can give significantly different results for similar structures in fixed and variable cell calculations.



(a) Original equation

(b) Corrected equation

FIG. 1: R-factor vs. perturbation size for an 8-atom unit cell, using (a) the original and (b) the corrected scattering intensities.

As a result of this error, structures of different volumes will give incorrect R-factors. This may have slowed the convergence of the GA calculations presented in the original paper.